

# High-resolution spectroscopy of gases at elevated temperatures

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# High-resolution spectroscopy of gases at elevated temperatures

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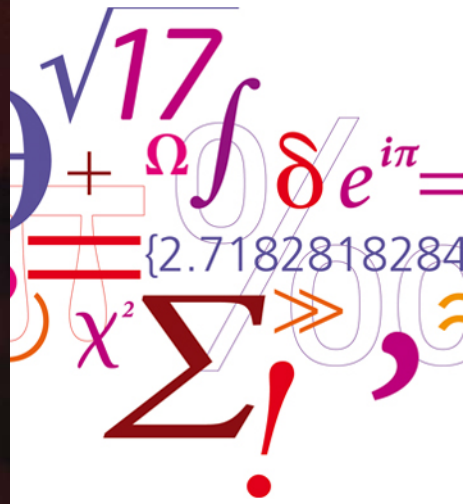


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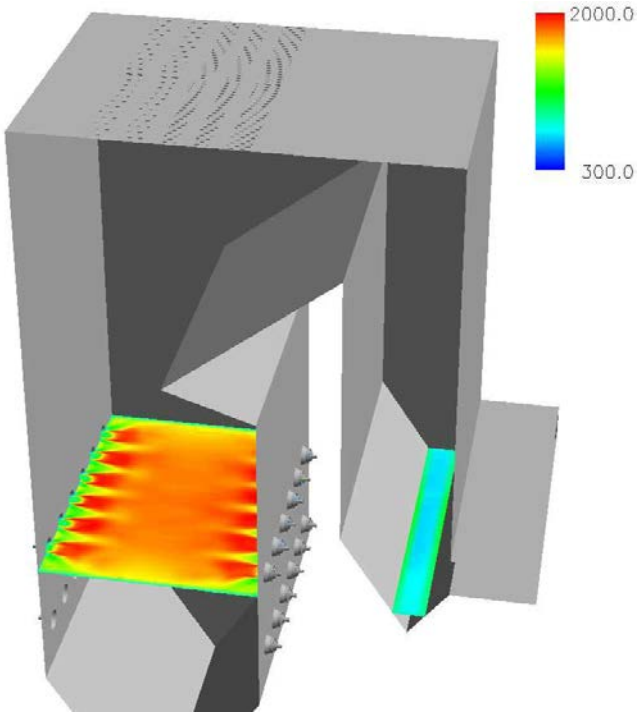
# Outline

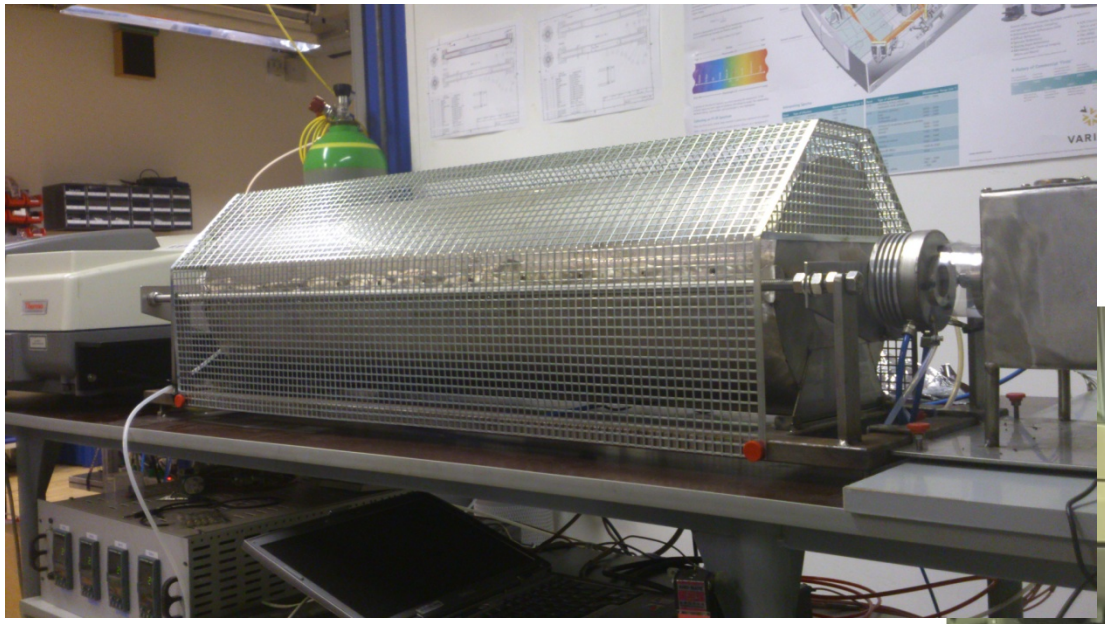
- Large scale measurements: why?
- Basic research: how it's made
- High resolution spectroscopy in flow gas cells: CO2(IR), SO2(one molecule: two applications) and Phenol(UV)
- SO3 project: the story
- Conclusions

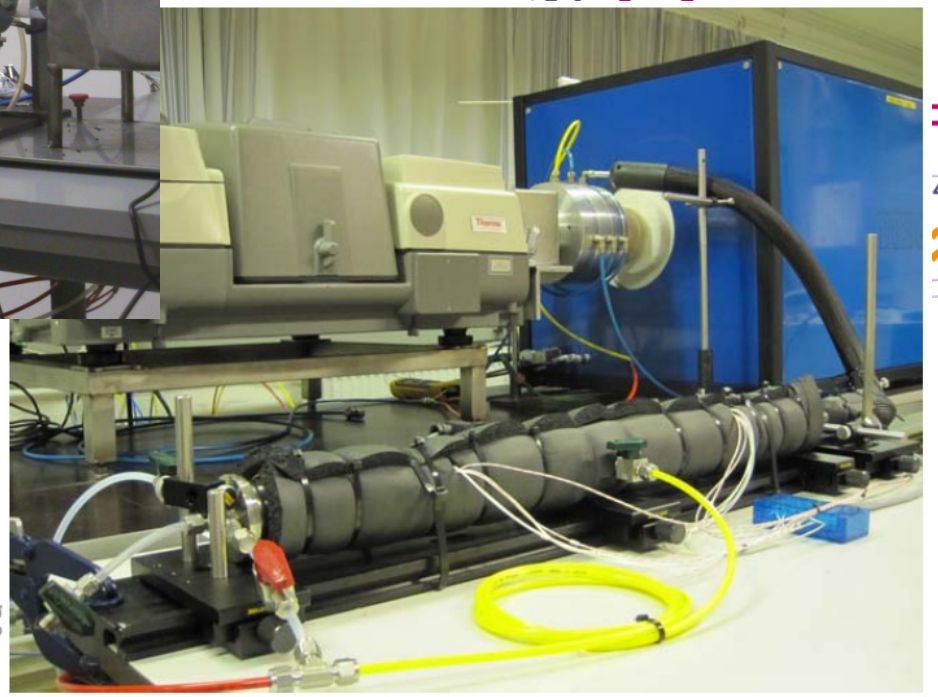
# Combustion: flames and hot flue gases




# Basic research

- focus on optical properties (TRS, ABS) of gases at temperatures up to 1600C;
- validation/building databases (e.g. HITRAN/HITEMP/CDSD…);
- various hot gas cells with highly-uniform temperature profiles (±0.5C).

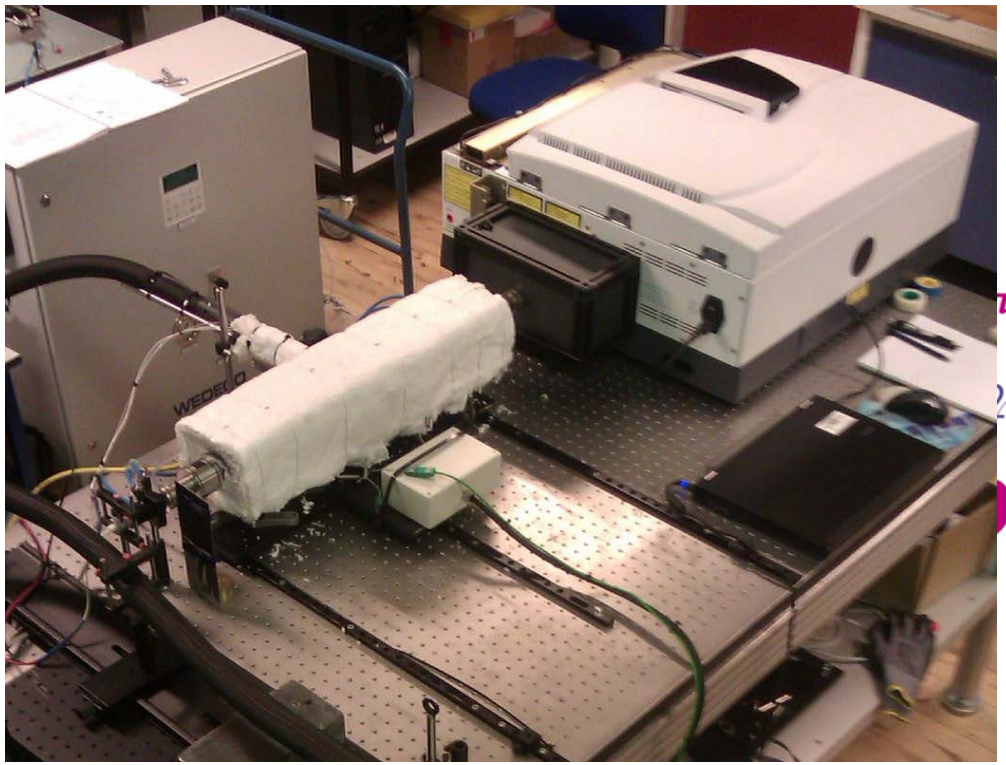




# Basic research

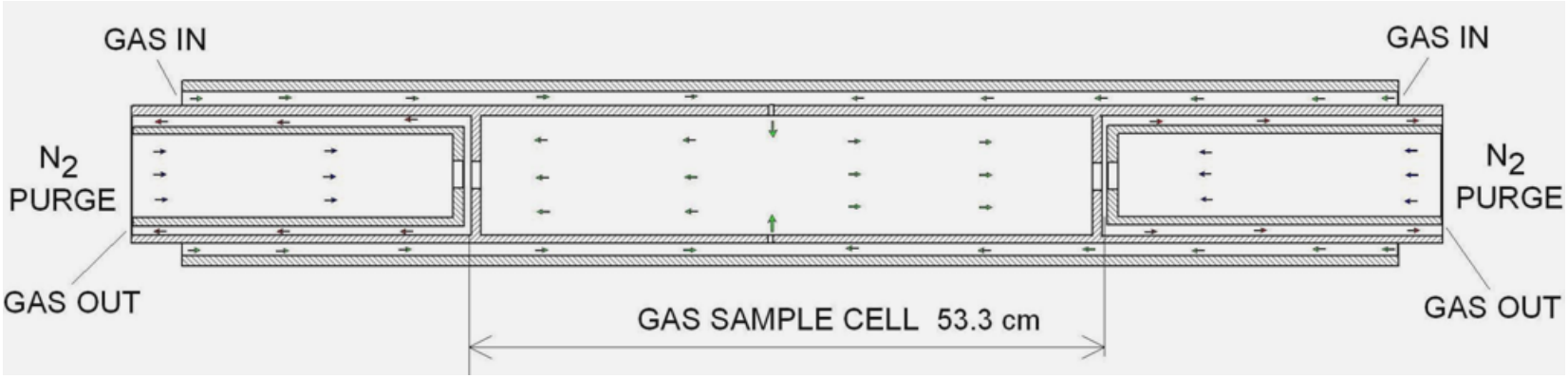
high-resolution spectroscopy (0.125 cm-1/0.016 nm) of “major” and “minor” (or trace) gases :

- CO2
- H2O
- SO2
- NH3
- SO3, H2S, OCS
- HCL, KCl, CH3Cl
- PAH’s,
- etc;



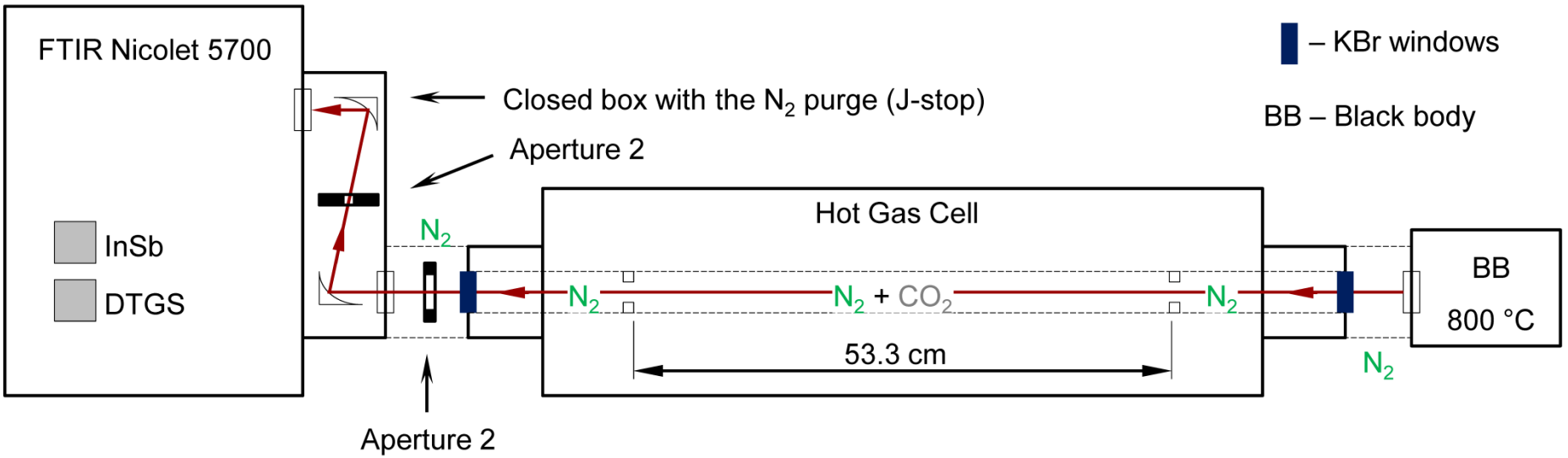
# Experimental set up: flow gas cell


- 3-zones gas cell;
- Non-windows;
- Highly-stable uniform T-profile (±0.5C);
- Tmax 1600C
- L=53.3 cm
- P=1 bar

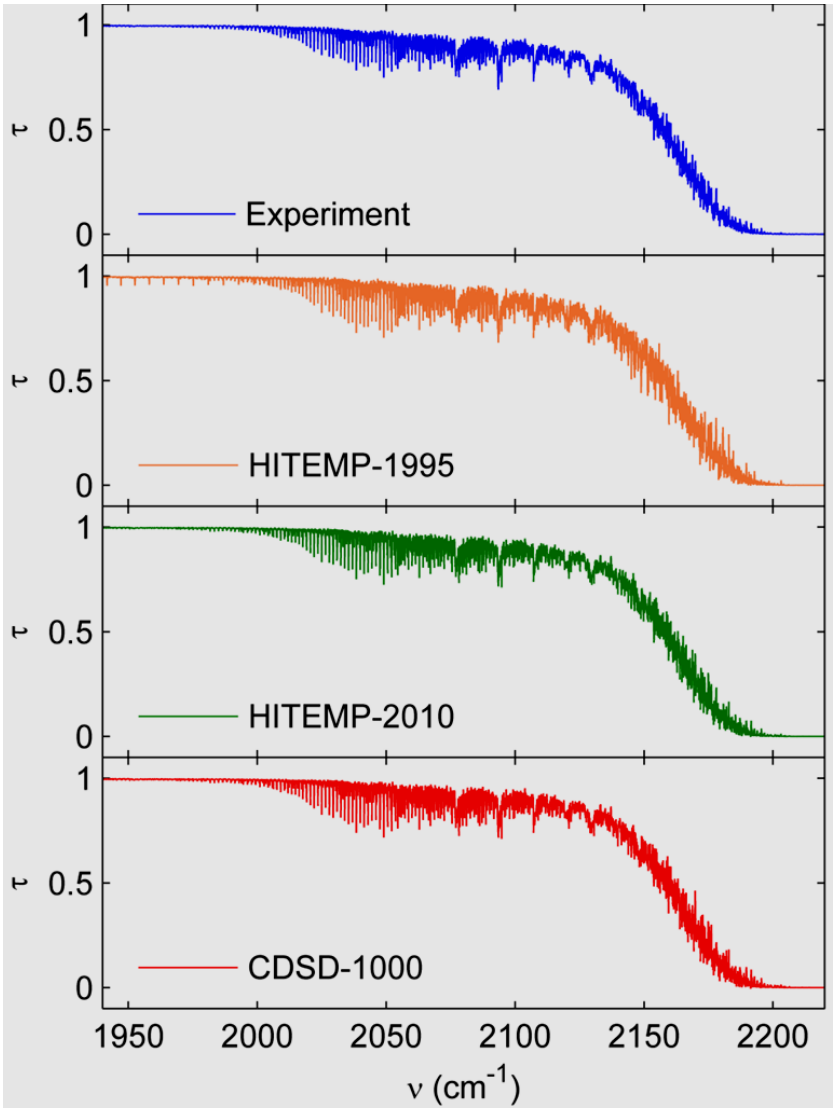


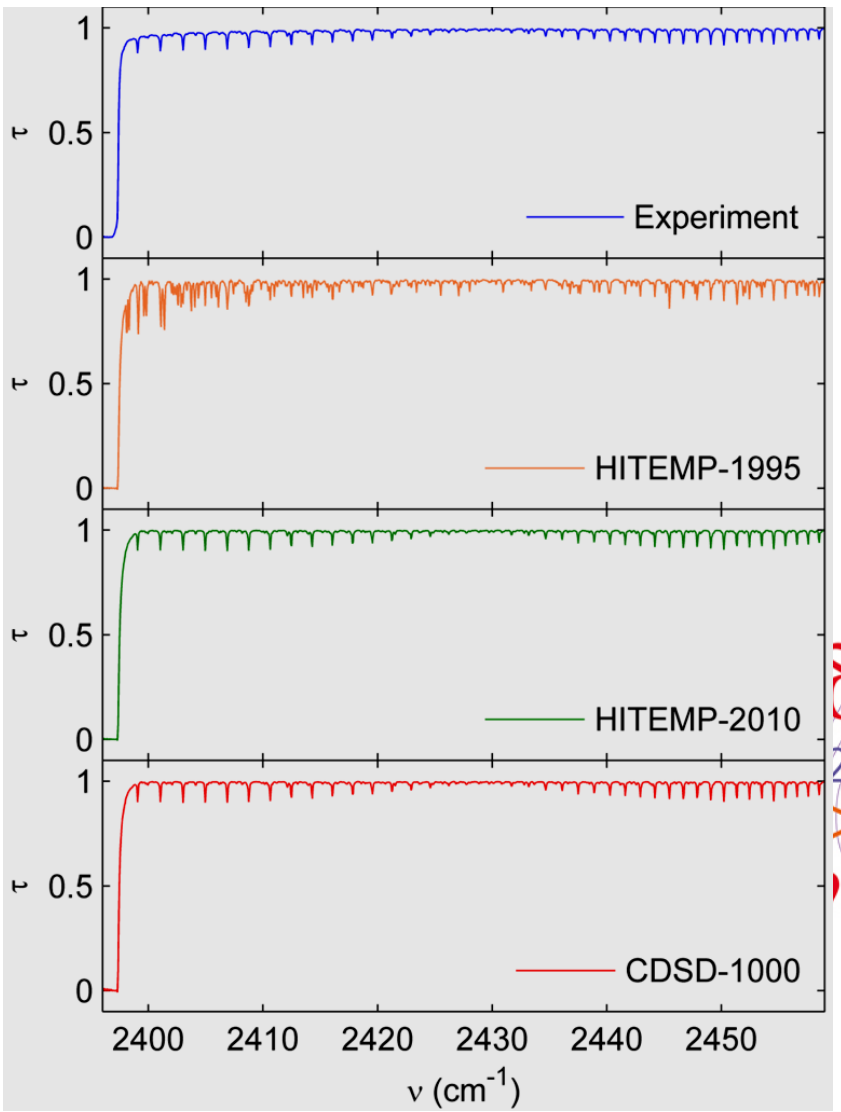
# Experimental set up: gas cell + FTIR spectrometer

Includes:
- a gas cell;
- a high-resolution FTIR spectrometer (Nicolet or Agilent);
- a light source (BB).

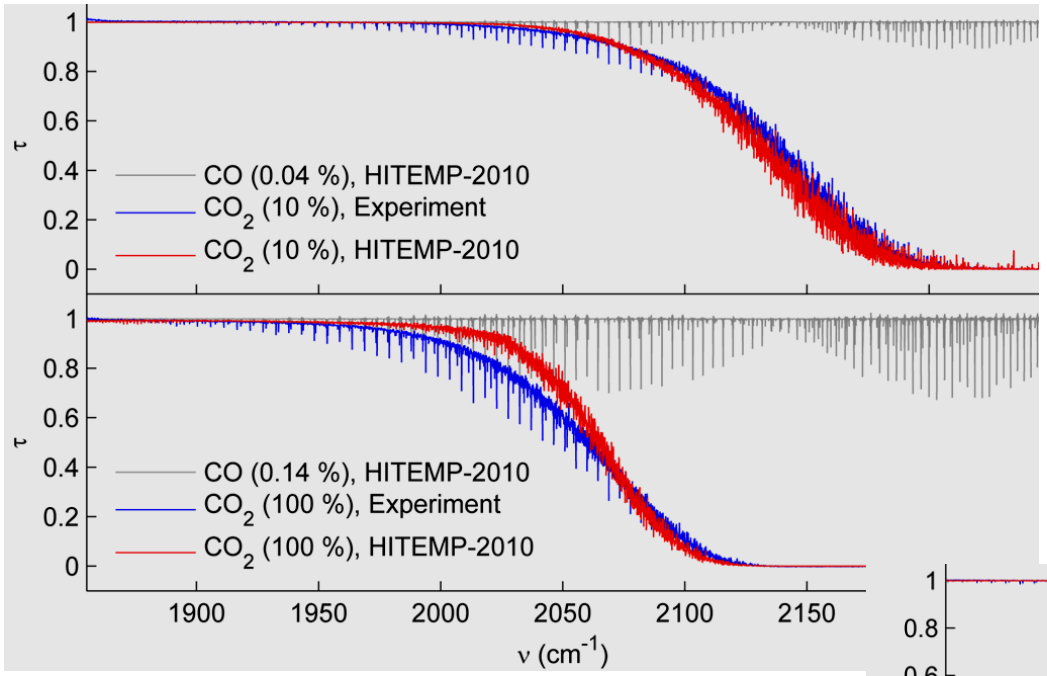


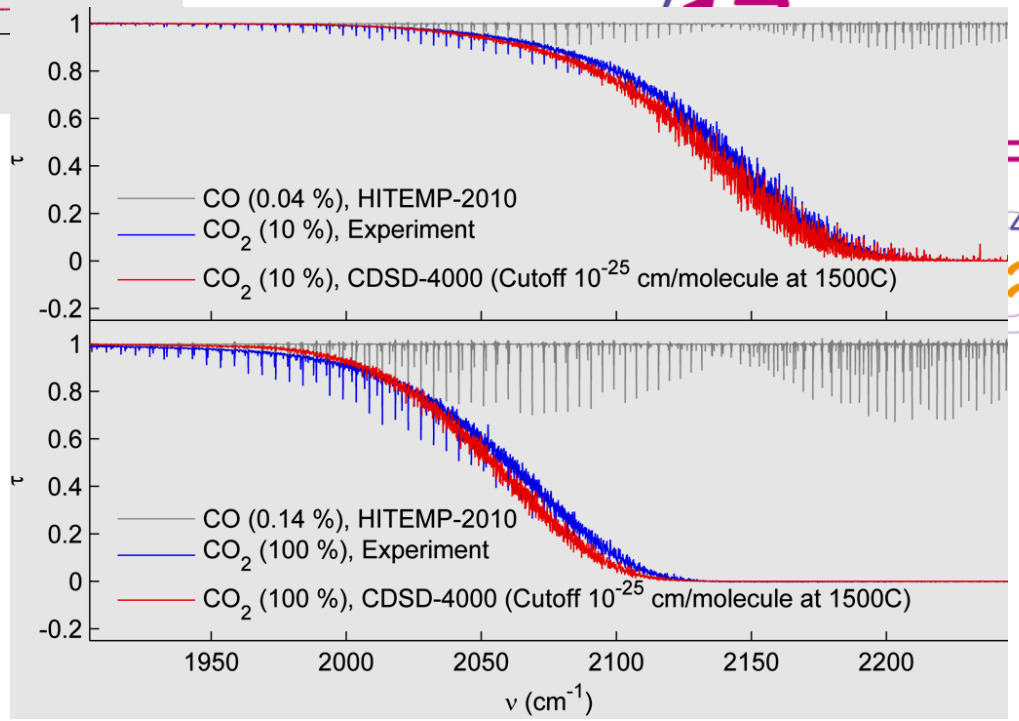
# CO2 transmission spectra: 727C



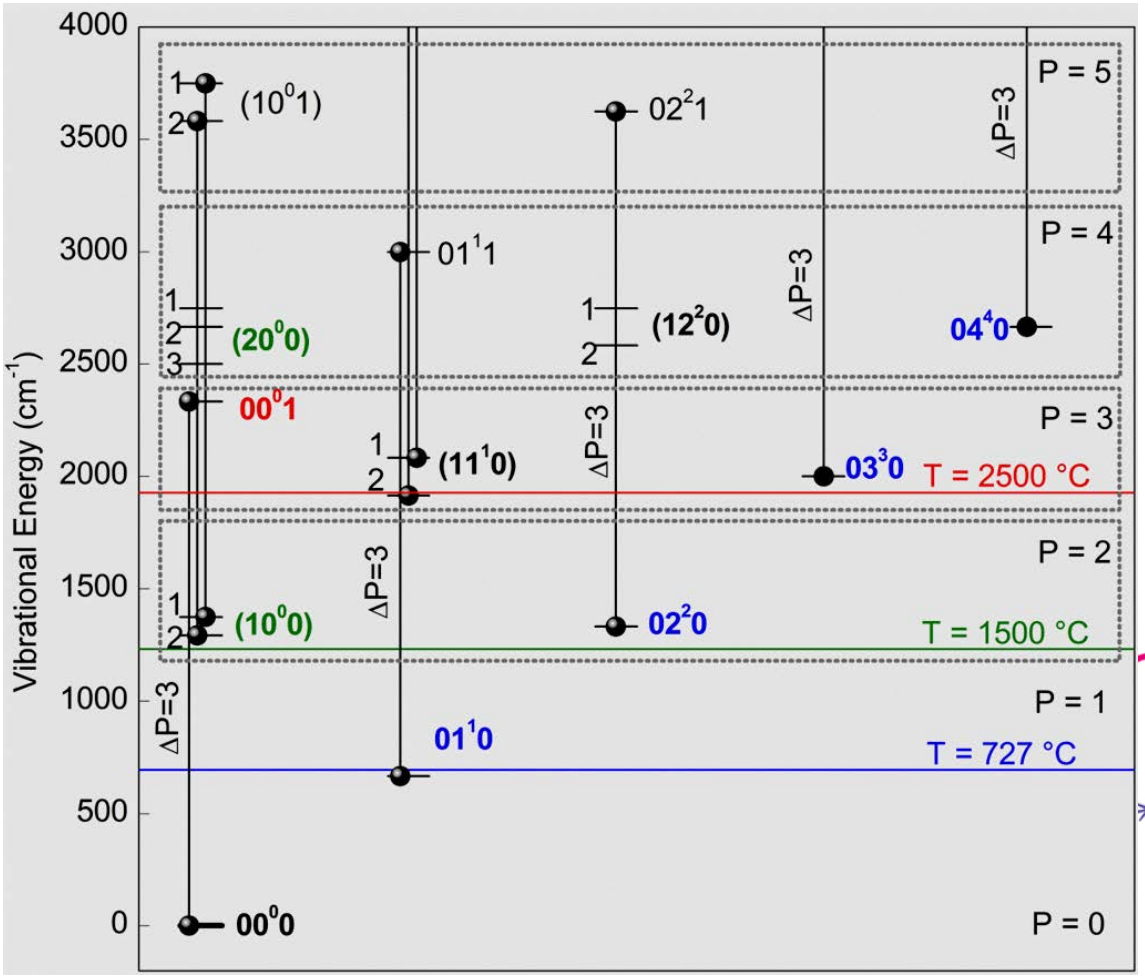



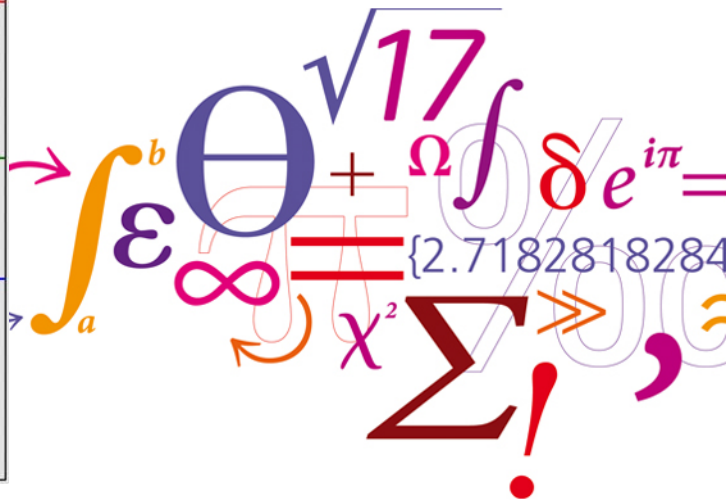
# CO2 transmission spectra: 1500C



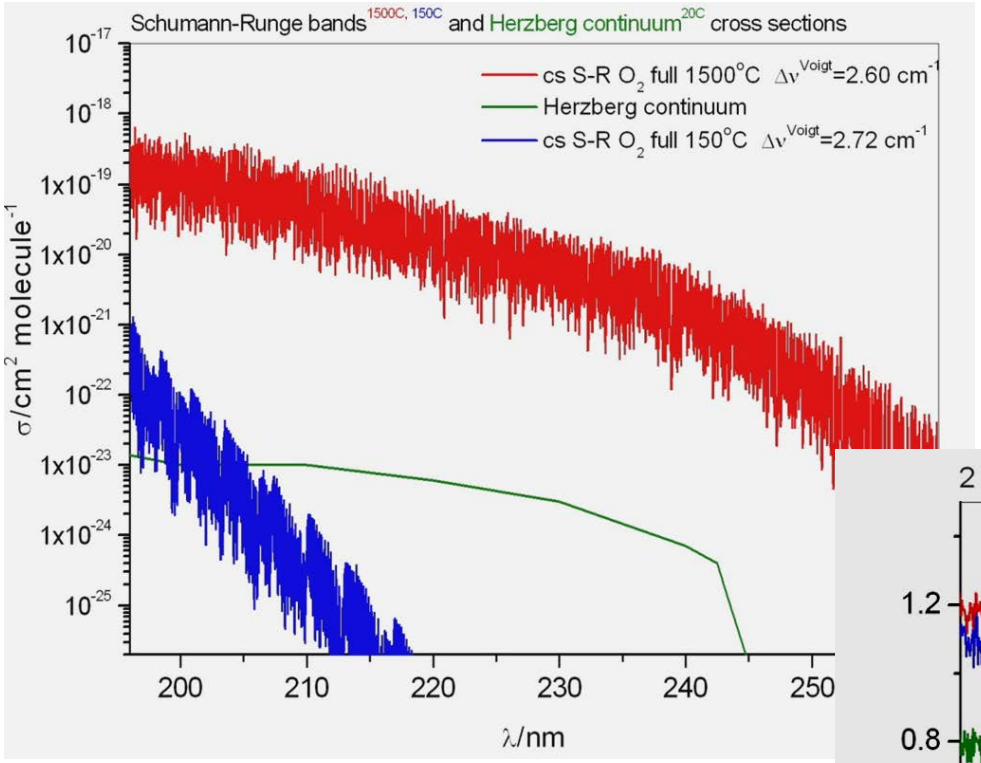
# CO2 quasicontinuum at 1500C



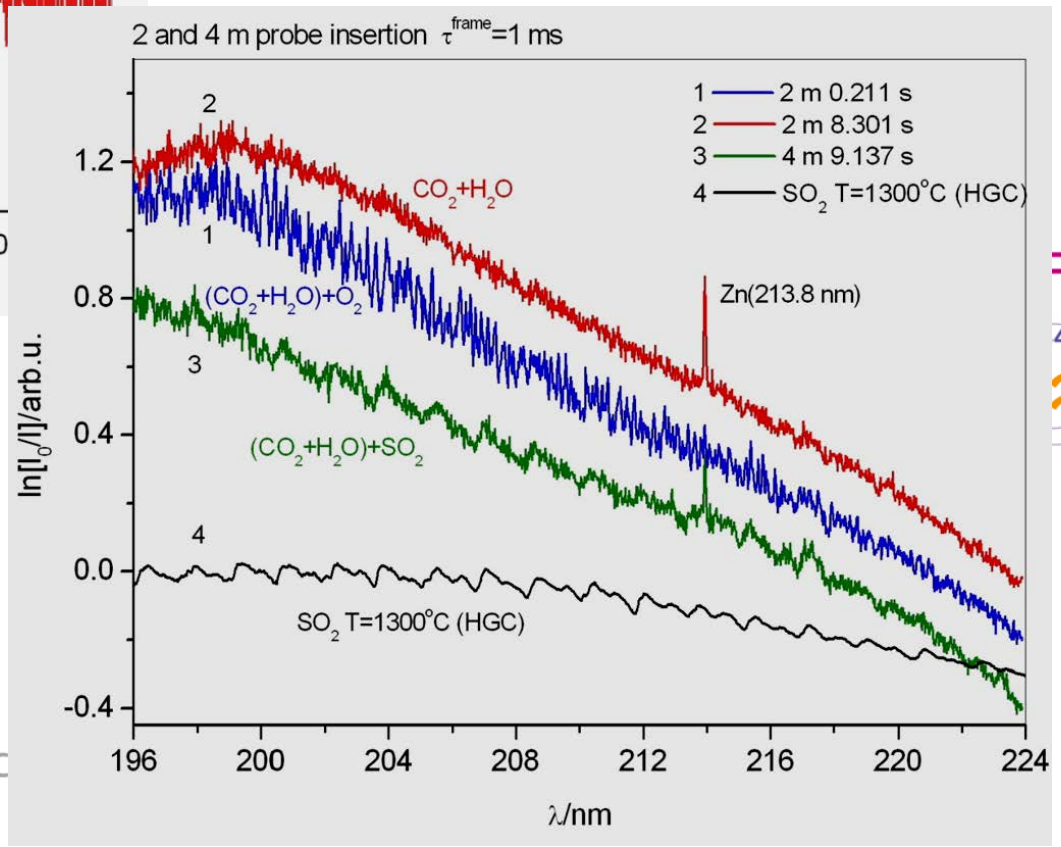
Details: JQSRT in press:
http://dx.doi.org/10.1016/j.jqsrt.2012.07.015

# SO2 spectroscopy: why?




O2 in turbulent flames:

- flame mapping
- mixing: combustion efficiency
- NOx chemistry
- fast (few ms) measurements

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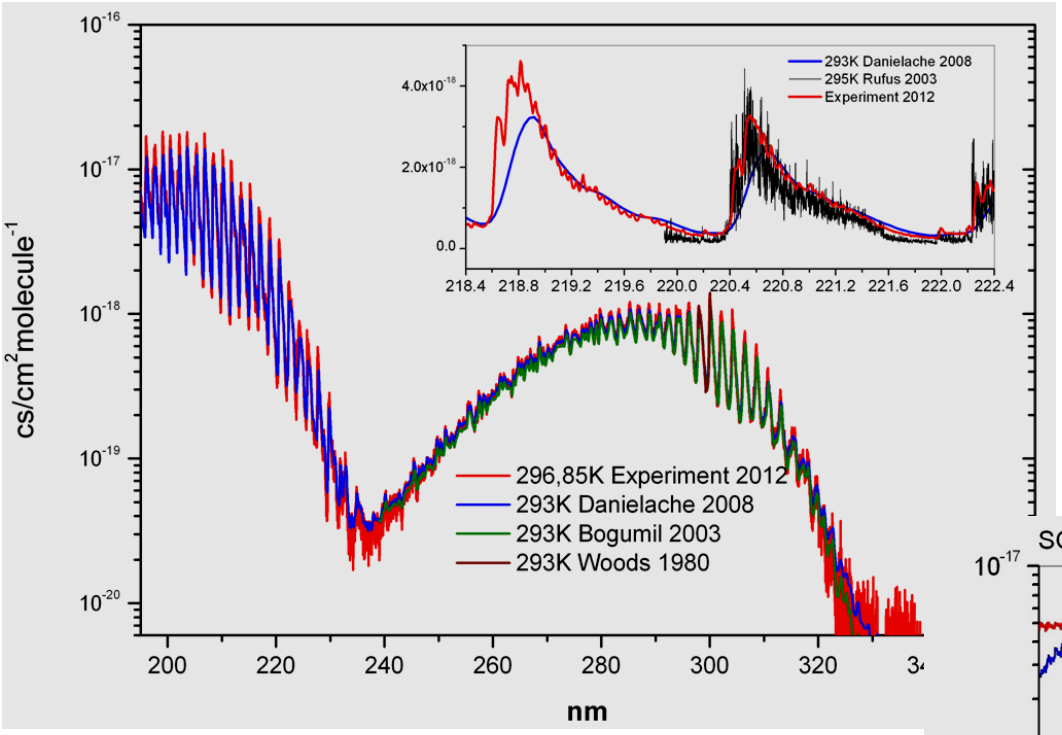
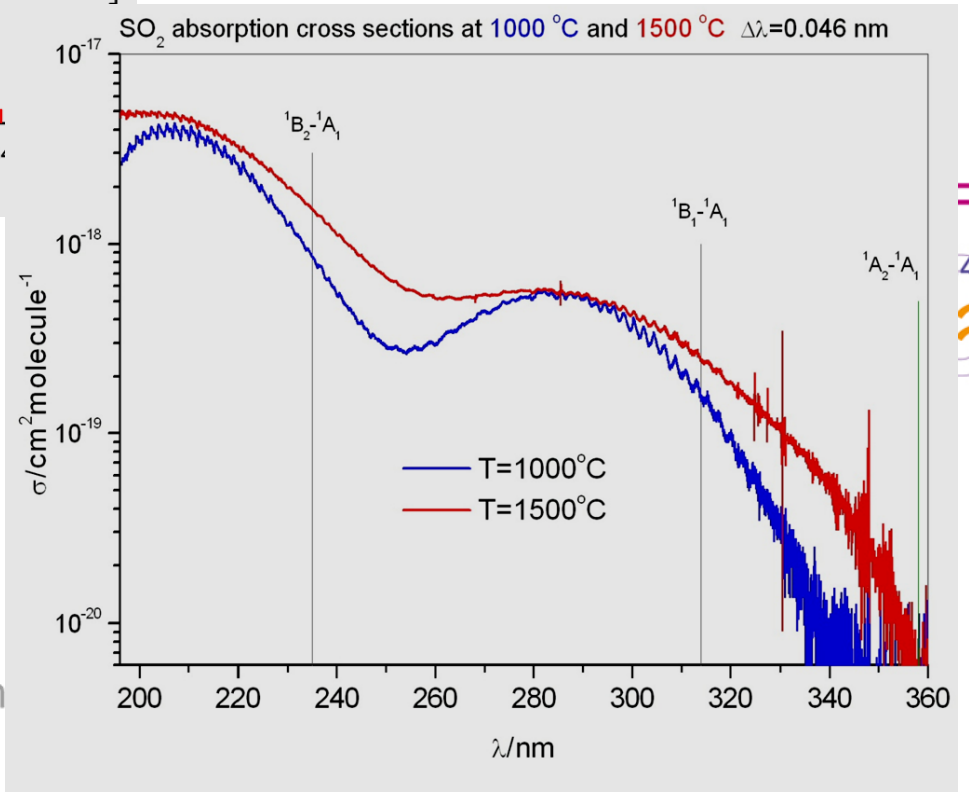
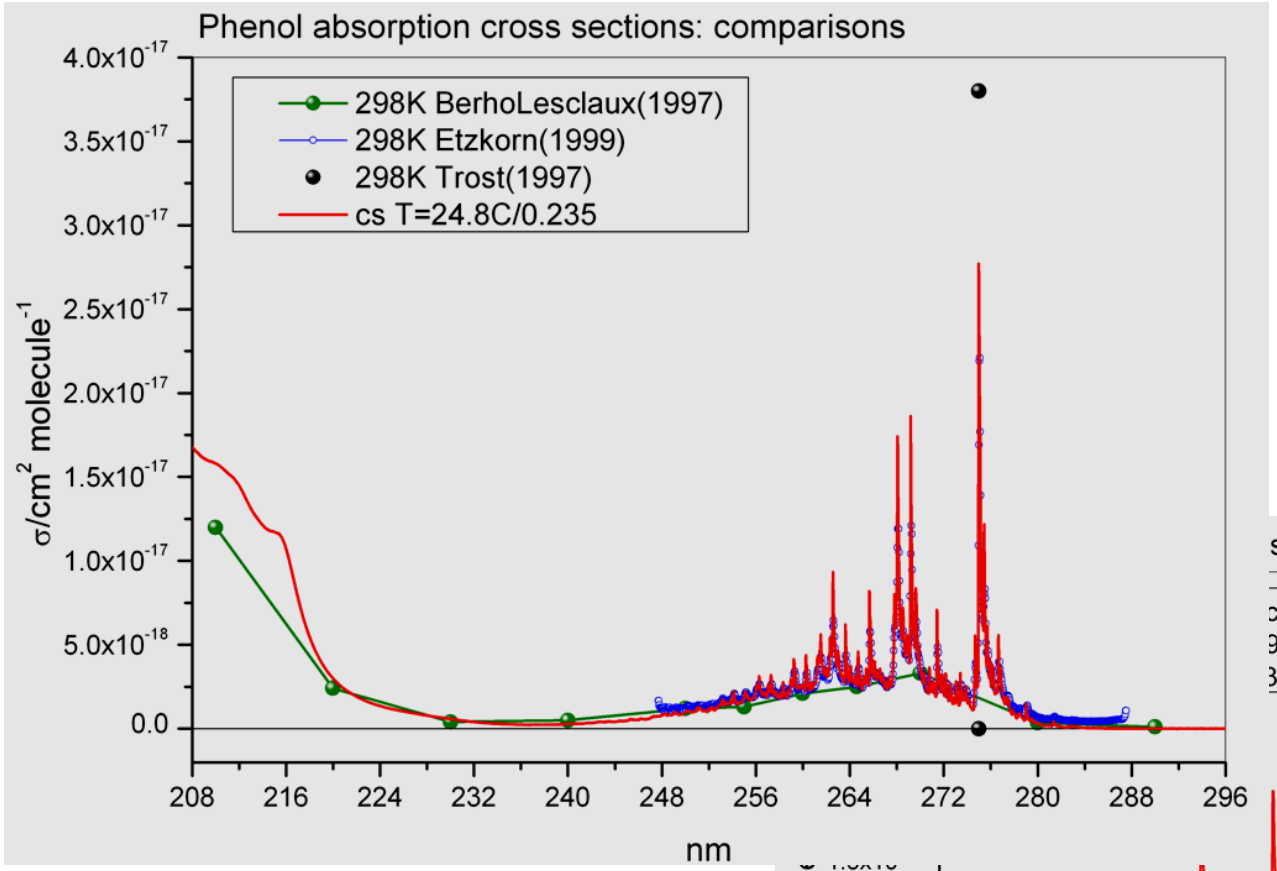
# SO2 spectroscopy: from validation to new data sets



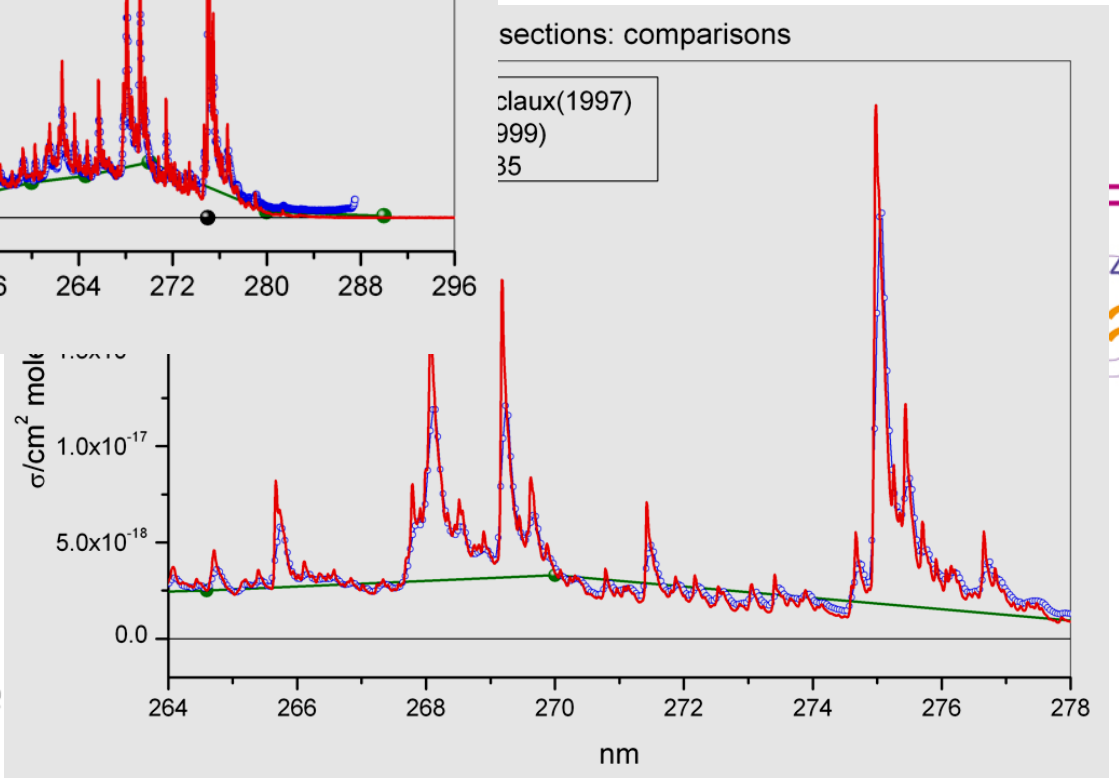



# Phenol spectroscopy: comparisons

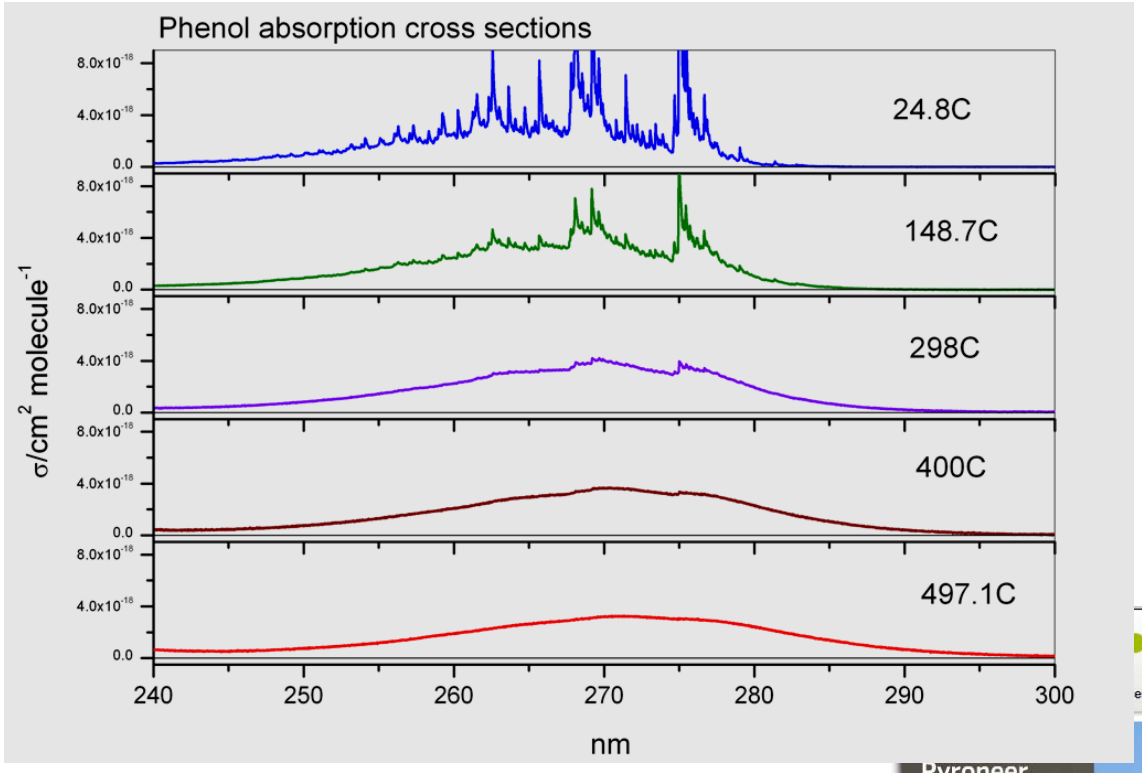



Phenol: solid to gas

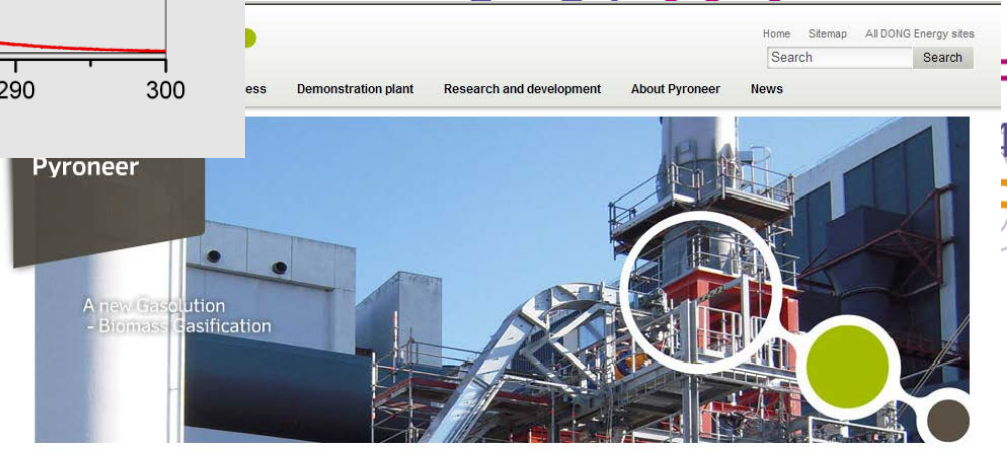
UV +GC/MS spectroscopy



# Phenol spectroscopy: temperature effects in LT-CFB gasification




- Producer gas:
  - corrosion (boilers)
  - reduced gas quality (fuel cells, gas grids)
- Phenol – major trace gas from PAH's in producer gas (LT-CFB process);
- Tgas about 550C;




See more:
http://www.dongenergy.com/pyroneer/Pages/index.aspx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# SO3 project: industry and university

**Facts:**

- Coal air combustion: SO2(300ppm) and SO3(5ppm) (blue smog);
- Large power plants: SCR units (NOx reduction) with NH3 injection;
- Global warming: operation at lower loads;
- Lower loads: lower gas temperatures at SCR units;
- By law: not allowed to turn off NH3 injection system.

**Problems:**

- Non optimal NH3 consumption;
- At lower T: H2SO4 formation which causes ammonia sulfate and ammonia bisulfate formation;

**Consequences:**

corrosion in ducts and plugging/damage of SCR elements.
costs: entire incidental costs a five day unit outage for SCR work could cost more than **$1 m** for a 500 MW unit

**Goal:**

to develop an optical method for SO3 ***in situ*** measurements.

# SO3 project: industry and university

Challenges of the project:

- temperature range 200-500C;
- SO3 high-resolution spectra (SO3 generation);
- SO2, NH3, H2SO4 and H2O high-resolution spectra database;

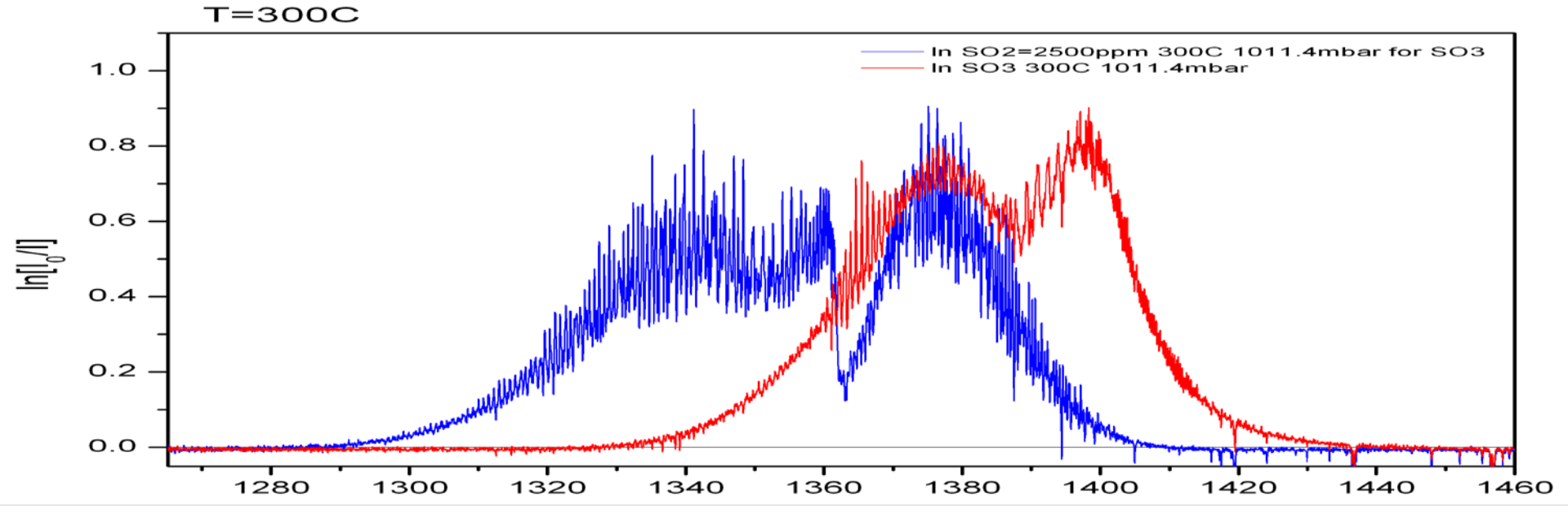
- water cooled optical probe development;
- powerful IR light source development;
- high sensitivity FTIR with linearized MCT or InSb detector;
- use of modern mathematical tools (e.g. SVD, NNLS).

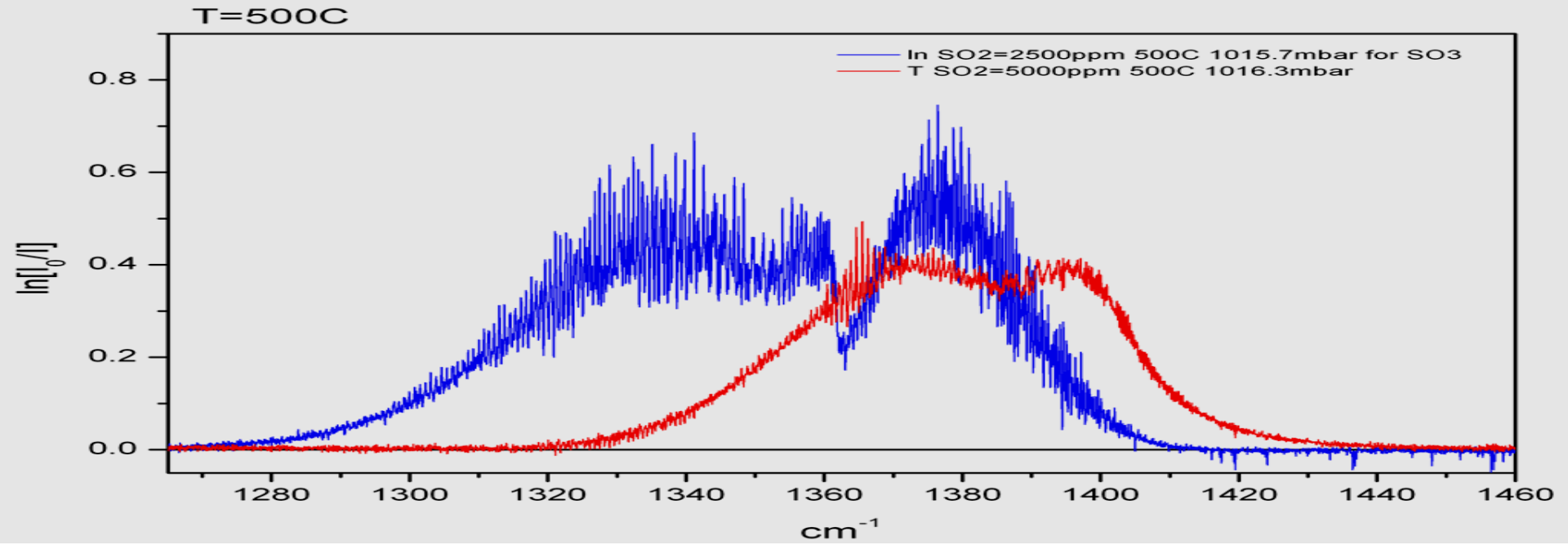
Two phases of the project:

- measurements in the lab and SO2/SO3 line list generation (UCL, UK)

- measurements on an industrial scale (power plant, Dong Energy, DK)

# SO3 project: high-resolution (0.115 cm-1) measurements



# Conclusions

High quality optical measurements with various gases (incl. highly corrosive gases) are possible;

A new gas cell is under development (<200 bar, 2000C)

Measurements can be used for: databases development and validation, studies of chemical reactions, energy exchange, validation of line shape models.

SO3 project is under development: lab work + PhD student employed by UCL;

Trace gases in gasification project is under development: lab work + PhD student employed by DTU

# Acknowledgements


- Energinet.dk: projects No. 2010-1-10622, 2010-1-10422
- Dong Energy
- UCL (Prof. Jonathan Tennyson)